вылете из решетки можно, используя стандартное выражение для флуктуации числа частиц [2] ферми-газа. Отклонение числа электронов от среднего и определяет заряд кластера Q. Вероятность получения заряда Q при вылете:

$$P_N(Q) = D_N^{-1} \exp\left(-2^{-1} Q^2 / \overline{\Delta Q_N^2}\right), \qquad \overline{\Delta Q_N^2} = e^2 \frac{3^{1/3}}{\pi^{5/3}} \frac{m_e T}{\hbar^2} \left(\frac{\overline{N_e}}{V}\right)^{1/3} \gamma^{1/3} N, \qquad (3)$$

где γ – число валентных электронов в атоме, T – температура решетки, а D_N - нормирующий множитель. Тогда вероятность покинуть решетку с определенной внутренней энергией и зарядом Q:

$$\frac{dW_N}{dE_{\text{int}}} P_N(Q)$$

Аналогичная процедура производится, чтобы узнать какой заряд g из кластера унесут испаряющиеся мономеры. При этом, температура вылетевшего кластера определяется через его внутреннюю энергию как $T_k = E_{\text{int}} / (3N - 6)$.

$$W_N^n(Q_0, g) = P_N(Q) \int_n^{(n+1)\delta} \frac{dW_N}{dE_{\text{int}}} P_n(g) dE_{\text{int}}$$

Суммируя это выражение по всем возможным значениям Q и g, получим выражение (1). Модель имеет хорошее согласие в области 4<N<80 для N-атомных металлических кластеров и ряда неметаллов.

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PROTECTION MECHANISM OF METAL SURFACE OXIDATION BY GRAPHENE

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Copper is widely used in electronics as an interconnecting material due to its high thermal and electrical conductivity. However, the formation of an oxide layer on the copper surface even at room temperature and resulting creation of trap states result in

significant degradation of its electronic, thermal, and interconnection capabilities. The earliest efforts to protect a metal from oxidation were to deposit carbon on metal surfaces, performed at elevated temperature. Graphene is not only the thinnest carbon material but also has exceptional mechanical and chemical stability. It adds a negligible thickness to the underlying metal while forming an electrically and thermally conductive coating. Graphene is also chemically inert in ambient atmosphere up to 400 °C and can be mechanically transferred to arbitrary surfaces. This remarkable chemical inertness is due to non-polar covalent carbon double bonds which prevent hydrogen bonding with water. The use of graphene as a corrosion barrier based on commercially available graphene-coated Cu has also been suggested. It has been recently found that deposition of graphene increases the thermal conductivity of 9-μm thick Cu film by up to 24% near room temperature. Such strong enhancement of Cu metal's thermal properties via graphene coating presents wide applications for graphene/Cu composites in fabrication of more robust electronic circuits. However, there is an alternative point of view suggesting that a graphene coating provides only short-term oxidation protection, and over long time scale it causes even more extensive wet corrosion. It is because the passivation property of graphene on Cu in ambient atmosphere still remains unclear.

Using method of comparing the calculated formation energies and experimental temperatures we can conclude that in the case of weakly oxidized graphene on a Cu substrate the vacancy formation will occur at temperatures around 200 °C. The obtained result is in qualitative agreement with experimental results of the observation of copper substrate oxidation after annealing of graphene/Cu systems [1].

We have demonstrated the properties of graphene as a protective layer for Cu. We have found from X-ray spectroscopic measurements that no evidence of electrochemical corrosion of copper covered by graphene after oxygen exposure at atmospheric pressure from 1 month to 1.5 years. The first-principles DFT calculations show that oxidation does not occur when the graphene monolayer is defect free. In the case of carbon vacancies, the interface of graphene/Cu becomes permeable to ingress of oxygen atoms, resulting in metal oxidation. Therefore, perfect graphene without defects or large grain boundaries can preserve the surface of copper from corrosion in ambient air over a long period of time.

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